Modeling and simulation of a multistage absorption hydration hybrid process using equation oriented modeling environment

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ABSTRACT

Separation of light hydrocarbon mixtures is one of the most important topics in chemical engineering research. With development of theories on hydrate equilibriums and kinetics, researchers are trying to apply hydration based separation technology to industrial applications. It is increasingly important to develop the corresponding simulation strategies for process design purposes. In this work we use an equation oriented modeling environment, named Aspen Custom Modeler® (ACM®), which enables rapid model development and provides powerful simulation solvers. With the help of ACM®, a multistage absorption hydration hybrid process (AHHP) for refinery dry gas separation is modeled and simulated. Sensitivities of key parameters such as water content and absorbent flow rate, are analyzed. Features of the multistage AHHP are discussed. For comparison, based on an industrial data, a butane absorption process is established and simulated. Economic evaluation shows that the multistage AHHP is competitive compared to current absorption process.

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1. Introduction

Separation of light hydrocarbon mixtures is one of the most important topics in chemical engineering research. Conventional methods for separating low boiling point gas mixture include cryogenic distillation and alkane absorption. New technologies such as reactive absorption, membrane separation and adsorption are investigated (Huang et al., 1999; Padin and Yang, 2000; Adhikari and Fernando, 2006). Recently, hydrate is proposed as a new tool for light hydrocarbon separations (Eslamimanesh et al., 2012).

1.1. Literature review on hydrate based separation experiment

Formed at high pressure and low temperature, hydrates are cage like, non-stoichiometric compounds composed of water and hydrocarbons (Sloan, 2003). When a mixture of hydrocarbons forms hydrate, some components are more easily captured than others. Large amount of work is performed in hydrate based light hydrocarbon separation. Ma et al. (2001, 2008) investigated the equilibriums of CH_4 and C_2H_4. Englezos et al. (1987a, 1987b) studied the kinetics of hydrate formation.

Recent research shows that for industrial purpose, forming hydrate with water as the continuous phase is unviable, because hydrate formed would float on top of water and thereby impede further hydration (H. Liu et al., 2013). Chen and coworkers put forward a new material named water in oil emulsion (w/o emulsion) and recommended it as the new absorbent (Turner et al., 2009; B. Liu et al., 2013; Ma et al., 2013a). Their observation shows hydrate agglomeration can be prevented, since hydrate generated is dispersed as tiny particles. Meanwhile, due to the large contact area between oil and water, hydration rate is facilitated (Mu et al., 2014).

Though excellent work is carried out by the scholars, literature survey shows current study has been focused on hydrate formation kinetics and equilibriums in single reactors. And there is a growing demand for a process scale modeling and simulation method which can provide insights and guidance for the further application of hydration technology.

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Symbols

A	Heat exchange area (m^2)
$\boldsymbol{C}$	Collection of components
C_j	Langmuir constants for component j
D	Vessel diameter (m)
f_j^L	Fugacity of j in liquid (bar)
f_j^V	Fugacity of j in vapor (bar)
H^{hy}	Molar enthalpy of hydrate (GJ/kmol)
H^L	Molar enthalpy of liquid (GJ/kmol)
H^V	Molar enthalpy of vapor (GJ/kmol)
HY_{in}	Hydrate mole flow rate going in (kmol/h)
HY_{out}	Hydrate mole leaving (kmol/h)
L	Vessel length (m)
L_{in}	Oil mole flow rate going in (kmol/h)
L_{out}	Oil mole flow rate leaving (kmol/h)
P	Pressure (bar)
P_0	Operating pressure (bar)
Q	Heat removed from stage (GJ)
T	Temperature (°C)
T_0	Operating temperature (°C)
V_{in}	Vapor mole flow rate going in (kmol/h)
V_{out}	Vapor mole flow rate leaving (kmol/h)
W_{cmp}	Working load of compressor (kW)
W^j	Mole flow rate of j in water (kmol/h)
x_{in}^j	Mole composition of oil liquid going in
x_{out}^j	Mole composition of oil liquid leaving
y_{in}^j	Mole composition of vapor going in
y_{out}^j	Mole composition of vapor leaving
z_{in}^j	Mole composition of hydrate going in
z_{out}^j	Mole composition of hydrate leaving

Table 1
FCC dry gas composition.

Component	Composition (mol%)
H_2	31.79
N_2	11.88
O_2	2.97
CO_2	2.01
CO	0.77
CH_4	24.65
C_2H_6	12.14
C_2H_4	12.56
C_3H_8	0.15
C_3H_6	1.05

Table 2
Operating condition of C4 absorption.

Unit operation	Pressure (MPa)	Temperature (°C)	Tray number
B-1	4.25	18	15
B-2	4.25	18–118	20
B-3	2.6	18–120	40
HX-1	2.6	In 120, out 40	–
HX-2	2.6	In 40, out 18	–
HX-3	2.6	In 40, out 18	–

increasingly important to recover ethylene from dry gas. A list of dry gas composition can be observed in Table 1 (Lei Si, 2013).

Admittedly, cryogenic distillation system is known to produce high quality products. However, at the same time, it also demands huge initial investment. As one of the most expensive units in cryogenic process, cold box is usually used to chill gas at cryogenic temperatures. To save investment in cold box, before cryogenic distillation, dry gas should be preprocessed, as is the case of Sheng Li refinery (Lei Si, 2013).

The C4 absorption flow chart for dry gas pretreatment can be observed in Fig. 1. The absorption flow chart can be divided into three parts: absorption (B-1), stripping (B-2) and desorption (B-3). Feed gas is absorbed in the absorption section. In stripping section, part of methane and nitrogen are driven away from the absorbent. Desorption column extracts enriched dry gas from butane. According to industrial data (Lei Si, 2013), the operating conditions are listed in Table 2. Pressure of enriched dry gas is 2.6 MPa. Before getting into cryogenic distillation, the enriched dry gas should be compressed up to 3.3 MPa, which is a typical condition for methane/ethylene separation (Salerno et al., 2011).

1.4. Contribution of this work

In this work, we build the models in Aspen Custom Modeler® (ACM), an integrated development environment for chemical process modeling (Aspen Technology, 2012). ACM can greatly reduce the amount of labor in coding by providing with the built in flash functions and property calculation procedures. The models are then exported as unit operation blocks to Aspen Plus® for integrated simulation and optimization.

Naeiji et al. (2014) proposed a multistage separation strategy for hydrate based separation. Following their footprints, we propose and simulate a multistage absorption hydration hybrid process (AHHP) for dry gas separation applications. Sensitivity of the key parameters are studied. Then we point out important features and evaluate some economic issues. For comparison, a C4 absorption process is also simulated and evaluated. It is found that the proposed AHHP is more economical. Reasons for the savings are discussed and analyzed. Nevertheless, we found there is still room for improvement provided that the refrigeration is reused.

To summarize, most previous work on hydration experiment and simulation is on unit operation scale. In this article we put

1.2. Literature review on hydration simulation

A number of theories are proposed for hydrate equilibrium calculation, among which Van-der-waals equations are the most famous. However, though accurately derived, solving the van-der-waals equations requires global optimization algorithm that is time consuming. As an alternative, Chen–Guo equations have a simpler formulation and can provide a quick solution without losing much accuracy, and thereby more appealing for process simulation purposes (Chen and Guo, 1998; Sloan and Koh, 2007).

Naeiji et al. (2014) calculated the performance of hydrate in separating methane and ethane with the help of a phase map. The phase map can provide an intuitive understanding in the hydration separation mechanism. Yet, there are two problems ahead for this method. First, the phase map cannot provide a quick and accurate solution. Second, it can only calculate the hydrate composition formed from pure water. Therefore, more robust simulation methods are needed.

1.3. Current process flow chart for dry gas separation

Ethylene is a fundamental raw material in petroleum industry. Refinery dry gas usually contains a significant amount of ethylene (about 10–20 mol%), which, however, is often flared for energy (Li and Luo, 2015). Moreover, the development in catalytic cracking, which primarily aimed to improve the light oil generation, results in ethylene content increment in dry gas (Rahimi and Karimzadeh, 2011; Sadeghbeigi, 2012). Therefore, it becomes